ELSEVIER

Chemical Physics 269 (2001) 447–450

Chemical Physics

www.elsevier.nl/locate/chemphys

Author index

Almeida, D.P., G. Dawber, S.E. Michelin and G.C. King, Core excitation and autoionising transitions from $^{1,3}\Pi_u$ states of N_2, by near threshold electron impact 269 (2001) 159
Ananthavel, S.P. and M. Manoharan, A theoretical study on electron donor–acceptor complexes of Et_2O, Et_2S and Me_3N with interhalogens, I–X (X = Cl and Br) 269 (2001) 49
Argyrakis, P., see Markovitsi, D. 269 (2001) 147

Bae, Y.C., see Jang, J.G. 269 (2001) 285
Bailey, W.C., Calculation of ^{14}N and ^{35}Cl quadrupole coupling constants on optimized molecular structures of pyrimidine, 2-X- and 5-X-pyrimidine, with X = F, Cl, Br, and CN 269 (2001) 75
Barić, D., see Maksić, Z.B. 269 (2001) 11
Becucci, M., see López-Tocón, I. 269 (2001) 29
Bignonneau, G., A. Fritsch and L. Ducasse, Non-orthogonal orbitals for localized electrons III. Application to periodic one dimensional lattices 269 (2001) 107
Bréchignac, P., see López-Tocón, I. 269 (2001) 29
Brion, C.E., J.B. Young, I.V. Litvinyuk and G. Cooper, An investigation of the HOMO frontier orbital electron density distributions of NH_3, the methylamines and NF_3 using DFT and electron momentum spectroscopy 269 (2001) 101

Castellucci, E., see López-Tocón, I. 269 (2001) 29
Čenský, M., see Jirásek, V. 269 (2001) 167
Chang, E.-C., see Hsu, J.-H. 269 (2001) 367
Chen, C., see Gao, Y. 269 (2001) 389
Chen, E.-S., see Hsu, J.-H. 269 (2001) 367
Chen, S.-A., see Hsu, J.-H. 269 (2001) 367
Chen, Y., see Gao, Y. 269 (2001) 389
Cooper, G., see Brion, C.E. 269 (2001) 101
Costa, S.M.B., see Ferreira, J.A.B. 269 (2001) 313

Dawber, G., see Almeida, D.P. 269 (2001) 159
Ding, H., see Güthe, F. 269 (2001) 347
Doetschman, D.C., see Gilbert, D.C. 269 (2001) 125
Domcke, W., see Ostojić, B. 269 (2001) 1
Došlić, N., J. Stare and J. Mavri, Hydrogen bonding in picolinic acid *N*-oxide. Part II: A proposal for dissipative laser driven proton transfer dynamics 269 (2001) 59
Ducasse, L., see Bignonneau, G. 269 (2001) 107

PII: S0301-0104(01)00389-5

Eerkens, J.W., Equilibrium dimer concentrations in gases and gas mixtures 269 (2001) 189
Egorov, V.V., On electrodynamics of extended multiphonon transitions and nature of the J-band 269 (2001) 251

Fann, W., see Hsu, J.-H. 269 (2001) 367
Feng, S.-y., see Zhou, Y.-f. 269 (2001) 441
Ferreira, J.A.B. and S.M.B. Costa, Thermally induced spectral diffusion of Rhodamine 3B in viscous polyols 269 (2001) 313
Francisco, J.S., see Guha, S. 269 (2001) 179
Fritsch, A., see Bignonneau, G. 269 (2001) 107
Fukuda, Y., see Hasegawa, M. 269 (2001) 323

Gadret, G., R. Zamboni, P. Schouwink, R.F. Mahrt, J. Thies, T. Loontjens and D.A. Leigh, Solid-state optical properties of the methyl-exopyridine–anthracene rotaxane 269 (2001) 381
Gallos, L.K., see Markovitsi, D. 269 (2001) 147
Gao, Y., Y. Chen, X. Ma and C. Chen, The collisional quenching of $CCl_2(A\,^1B_1$ and $a\,^3B_1)$ by substituted methane molecules 269 (2001) 389
Gilbert, D.C. and D.C. Doetschman, Five-coordinate nitrosyl iron(II) tetraphenylporphyrin exhibits porphyrin ring ^{14}N symmetry about the Fe–N–O plane: a hyperfine sublevel correlation spectroscopy study 269 (2001) 125
Guha, S. and J.S. Francisco, A theoretical study of the reaction of hypochlorous acid with the bromite ion 269 (2001) 179
Gulbinas, V., see Karpicz, R. 269 (2001) 357
Güthe, F., H. Ding, T. Pino and J.P. Maier, Diagnosis of a benzene discharge with a mass-selective spectroscopic technique 269 (2001) 347

Hackbarth, S., V. Horneffer, A. Wiehe, F. Hillenkamp and B. Röder, Photophysical properties of pheophorbide-*a*-substituted diaminobutane poly-propylene-imine dendrimer 269 (2001) 339
Hasegawa, M., A. Nakao, M. Masui, T. Tamura, D. Suzuki, W. Linert, Y. Fukuda and T. Hoshi, Higher excited state fluorescence of mixed ligand lanthanide(III) complexes with acetylacetonato, nitrate and terpyridine 269 (2001) 323
Hillenkamp, F., see Hackbarth, S. 269 (2001) 339
Horneffer, V., see Hackbarth, S. 269 (2001) 339
Hornowski, T. and D. Madej, Ultrasonic studies of dynamics of critical concentration fluctuations in benzonitrile–isooctane mixture 269 (2001) 303
Hoshi, T., see Hasegawa, M. 269 (2001) 323
Hsu, J.-H., W. Fann, H.-F. Meng, E.-S. Chen, E.-C. Chang, S.-A. Chen and K.-W. To, Decay dynamics of interchain excited states in luminescent conjugated polymer CN-PPV 269 (2001) 367

Jang, J.G. and Y.C. Bae, Vapor–liquid equilibria of dendrimer solutions: the effect of endgroups at the periphery of dendrimer molecules 269 (2001) 285
Jiang, M.-h., see Zhou, Y.-f. 269 (2001) 441
Jirásek, V., O. Špalek, J. Kodymová and M. Čenský, Chemical generation of atomic iodine for chemical oxygen–iodine laser. I. Modelling of reaction systems 269 (2001) 167

Karamanis, P., see Maroulis, G. 269 (2001) 137
Karpicz, R., V. Gulbinas, A. Stanishauskaite and A. Undzenas, Characterization of bisazo compounds employing ultrafast spectroscopy 269 (2001) 357

Kim, H.-S., A Monte Carlo simulation study of solvent effect on Eu^{3+} to Nd^{3+} ion mutation 269 (2001) 295
King, G.C., see Almeida, D.P. 269 (2001) 159
Klokishner, S., Cobalt valence tautomeric compounds: molecular and solid state properties 269 (2001) 411
Kodymová, J., see Jirásek, V. 269 (2001) 167
Kummer, A.D., see Voityuk, A.A. 269 (2001) 83

Leigh, D.A., see Gadret, G. 269 (2001) 381
Lemaistre, J.P., see Markovitsi, D. 269 (2001) 147
Linert, W., see Hasegawa, M. 269 (2001) 323
Litvinyuk, I.V., see Brion, C.E. 269 (2001) 101
Loontjens, T., see Gadret, G. 269 (2001) 381
López-Tocón, I., J.C. Otero, M. Becucci, G. Pietraperzia, E. Castellucci and P. Bréchignac, Potential coupling of intramolecular to intermolecular modes: an ab initio study of the amino inversion and van der Waals motions in the aniline–argon complex 269 (2001) 29

Ma, X., see Gao, Y. 269 (2001) 389
Madej, D., see Hornowski, T. 269 (2001) 303
Mahrt, R.F., see Gadret, G. 269 (2001) 381
Maier, J.P., see Güthe, F. 269 (2001) 347
Maksić, Z.B., D.M. Smith and D. Barić, The additivity of the π-electron correlation energy in planar heteroatomic molecules 269 (2001) 11
Manoharan, M., see Ananthavel, S.P. 269 (2001) 49
Markovitsi, D., L.K. Gallos, J.P. Lemaistre and P. Argyrakis, Degeneracy, orientational disorder and chromophore size effects on Frenkel excitons in columnar mesophases 269 (2001) 147
Maroulis, G. and P. Karamanis, Finite-field Møller–Plesset perturbation theory and coupled cluster calculations of the electric multipole moments and the dipole polarizability of As_2 269 (2001) 137
Masui, M., see Hasegawa, M. 269 (2001) 323
Mavri, J., see Došlić, N. 269 (2001) 59
Meng, F.-q., see Zhou, Y.-f. 269 (2001) 441
Meng, H.-F., see Hsu, J.-H. 269 (2001) 367
Michel-Beyerle, M.-E., see Voityuk, A.A. 269 (2001) 83
Michelin, S.E., see Almeida, D.P. 269 (2001) 159

Nakao, A., see Hasegawa, M. 269 (2001) 323

Ostojić, B. and W. Domcke, Ab initio investigation of the potential energy surfaces involved in the photophysics of s-*trans*-1,3-butadiene 269 (2001) 1
Otero, J.C., see López-Tocón, I. 269 (2001) 29

Penzkofer, A., see Zweck, J. 269 (2001) 399
Pietraperzia, G., see López-Tocón, I. 269 (2001) 29
Pino, T., see Güthe, F. 269 (2001) 347

Röder, B., see Hackbarth, S. 269 (2001) 339
Rösch, N., see Voityuk, A.A. 269 (2001) 83

Schouwink, P., see Gadret, G. 269 (2001) 381
Smith, D.M., see Maksić, Z.B. 269 (2001) 11
Špalek, O., see Jirásek, V. 269 (2001) 167
Stanishauskaite, A., see Karpicz, R. 269 (2001) 357
Stare, J., see Došlić, N. 269 (2001) 59
Suzuki, D., see Hasegawa, M. 269 (2001) 323

Takayanagi, T. and A. Wada, Reduced dimensionality quantum reactive scattering calculations on the ab initio potential energy surface for the $O(^1D) + N_2O \rightarrow NO + NO$ reaction 269 (2001) 37
Tamura, T., see Hasegawa, M. 269 (2001) 323
Thies, J., see Gadret, G. 269 (2001) 381
To, K.-W., see Hsu, J.-H. 269 (2001) 367

Undzenas, A., see Karpicz, R. 269 (2001) 357

Voityuk, A.A., A.D. Kummer, M.-E. Michel-Beyerle and N. Rösch, Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results 269 (2001) 83

Wada, A., see Takayanagi, T. 269 (2001) 37
Wiehe, A., see Hackbarth, S. 269 (2001) 339
Wu, G., The influence of the stretch modes on the classical highly excited bend motion with Darling–Dennison coupling in acetylene 269 (2001) 93

Xiong, R.-g., see Zhu, X.-l. 269 (2001) 243

You, X.-z., see Zhu, X.-l. 269 (2001) 243
Young, J.B., see Brion, C.E. 269 (2001) 101

Zamboni, R., see Gadret, G. 269 (2001) 381
Zhao, X., see Zhou, Y.-f. 269 (2001) 441
Zhou, Z., see Zhu, X.-l. 269 (2001) 243
Zhou, Y.-f., F.-q. Meng, X. Zhao, S.-y. Feng and M.-h. Jiang, Theoretical study TPA properties of a series of two-dimensional charge-transfer derivatives 269 (2001) 441
Zhu, X.-l., X.-z. You, R.-g. Xiong and Z. Zhou, Molecular dynamics studies of phase transition of KI clusters 269 (2001) 243
Zweck, J. and A. Penzkofer, Microstructure of indocyanine green J-aggregates in aqueous solution 269 (2001) 399

ELSEVIER

Chemical Physics 269 (2001) 451–461

Chemical Physics

www.elsevier.nl/locate/chemphys

Subject index

Methods and constructs

Theoretical

Computational methods for electronic structure

Ab initio investigation of the potential energy surfaces involved in the photophysics of s-*trans*-1,3-butadiene, B. Ostojić and W. Domcke 269 (2001) 1

The additivity of the π-electron correlation energy in planar heteroatomic molecules, Z.B. Maksić, D.M. Smith and D. Barić 269 (2001) 11

Calculation of ^{14}N and ^{35}Cl quadrupole coupling constants on optimized molecular structures of pyrimidine, 2-X- and 5-X-pyrimidine, with X = F, Cl, Br, and CN, W.C. Bailey 269 (2001) 75

-CI and valence bond approach

Theoretical study TPA properties of a series of two-dimensional charge-transfer derivatives, Y.-f. Zhou, F.-q. Meng, X. Zhao, S.-y. Feng and M.-h. Jiang 269 (2001) 441

-perturbative and many body approaches

The additivity of the π-electron correlation energy in planar heteroatomic molecules, Z.B. Maksić, D.M. Smith and D. Barić 269 (2001) 11

Potential coupling of intramolecular to intermolecular modes: an ab initio study of the amino inversion and van der Waals motions in the aniline–argon complex, I. López-Tocón, J.C. Otero, M. Becucci, G. Pietraperzia, E. Castellucci and P. Bréchignac 269 (2001) 29

Reduced dimensionality quantum reactive scattering calculations on the ab initio potential energy surface for the $O(^1D) + N_2O \rightarrow NO + NO$ reaction, T. Takayanagi and A. Wada 269 (2001) 37

-density functional theory

A theoretical study on electron donor–acceptor complexes of Et_2O, Et_2S and Me_3N with interhalogens, I–X (X = Cl and Br), S.P. Ananthavel and M. Manoharan 269 (2001) 49

Hydrogen bonding in picolinic acid *N*-oxide. Part II: A proposal for dissipative laser driven proton transfer dynamics, N. Došlić, J. Stare and J. Mavri 269 (2001) 59

Calculation of ^{14}N and ^{35}Cl quadrupole coupling constants on optimized molecular structures of pyrimidine, 2-X- and 5-X-pyrimidine, with X = F, Cl, Br, and CN, W.C. Bailey 269 (2001) 75

PII: S0301-0104(01)00390-1

Semiempirical methods
Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results, A.A. Voityuk, A.D. Kummer, M.-E. Michel-Beyerle and N. Rösch 269 (2001) 83
Theoretical study TPA properties of a series of two-dimensional charge-transfer derivatives, Y.-f. Zhou, F.-q. Meng, X. Zhao, S.-y. Feng and M.-h. Jiang 269 (2001) 441

Algebraic approaches
The influence of the stretch modes on the classical highly excited bend motion with Darling–Dennison coupling in acetylene, G. Wu 269 (2001) 93

Wavefunctions for highly excited and unbound states
An investigation of the HOMO frontier orbital electron density distributions of NH_3, the methylamines and NF_3 using DFT and electron momentum spectroscopy, C.E. Brion, J.B. Young, I.V. Litvinyuk and G. Cooper 269 (2001) 101

Spin states and magnetic interactions
Non-orthogonal orbitals for localized electrons III. Application to periodic one dimensional lattices, G. Bignonneau, A. Fritsch and L. Ducasse 269 (2001) 107
Five-coordinate nitrosyl iron(II) tetraphenylporphyrin exhibits porphyrin ring ^{14}N symmetry about the Fe–N–O plane: a hyperfine sublevel correlation spectroscopy study, D.C. Gilbert and D.C. Doetschman 269 (2001) 125

Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)
Finite-field Møller–Plesset perturbation theory and coupled cluster calculations of the electric multipole moments and the dipole polarizability of As_2, G. Maroulis and P. Karamanis 269 (2001) 137

Photon states and statistics
Degeneracy, orientational disorder and chromophore size effects on Frenkel excitons in columnar mesophases, D. Markovitsi, L.K. Gallos, J.P. Lemaistre and P. Argyrakis 269 (2001) 147

Scattering of waves and particles
Core excitation and autoionising transitions from $^{1,3}\Pi_u$ states of N_2, by near threshold electron impact, D.P. Almeida, G. Dawber, S.E. Michelin and G.C. King 269 (2001) 159

Collisional and reactive molecular dynamics with non-frictional forces
Reduced dimensionality quantum reactive scattering calculations on the ab initio potential energy surface for the $O(^1D) + N_2O \rightarrow NO + NO$ reaction, T. Takayanagi and A. Wada 269 (2001) 37
Chemical generation of atomic iodine for chemical oxygen–iodine laser. I. Modelling of reaction systems, V. Jirásek, O. Špalek, J. Kodymová and M. Čenský 269 (2001) 167

Reactive molecular dynamics including dissipative processes
A theoretical study of the reaction of hypochlorous acid with the bromite ion, S. Guha and J.S. Francisco 269 (2001) 179

Intramolecular dynamics
Hydrogen bonding in picolinic acid *N*-oxide. Part II: A proposal for dissipative laser driven proton transfer dynamics, N. Došlić, J. Stare and J. Mavri 269 (2001) 59
The influence of the stretch modes on the classical highly excited bend motion with Darling–Dennison coupling in acetylene, G. Wu 269 (2001) 93

Molecular dynamics of many particle systems and condensed phases
Equilibrium dimer concentrations in gases and gas mixtures, J.W. Eerkens 269 (2001) 189
Molecular dynamics studies of phase transition of KI clusters, X.-l. Zhu, X.-z. You, R.-g. Xiong and Z. Zhou 269 (2001) 243

Quasiparticle dynamics (incl. excitons, polarons)
On electrodynamics of extended multiphonon transitions and nature of the J-band, V.V. Egorov 269 (2001) 251

Migration and interaction on grids and lattices
Vapor–liquid equilibria of dendrimer solutions: the effect of endgroups at the periphery of dendrimer molecules, J.G. Jang and Y.C. Bae 269 (2001) 285

Statistical computational methods (incl. Monte Carlo)
A Monte Carlo simulation study of solvent effect on Eu^{3+} to Nd^{3+} ion mutation, H.-S. Kim 269 (2001) 295

Equilibrium statistical mechanics and thermodynamics
A Monte Carlo simulation study of solvent effect on Eu^{3+} to Nd^{3+} ion mutation, H.-S. Kim 269 (2001) 295

Theory of critical behavior
Ultrasonic studies of dynamics of critical concentration fluctuations in benzonitrile–isooctane mixture, T. Hornowski and D. Madej 269 (2001) 303

Time and space correlation functions
Thermally induced spectral diffusion of Rhodamine 3B in viscous polyols, J.A.B. Ferreira and S.M.B. Costa 269 (2001) 313

Experiment

Magnetic resonances
Five-coordinate nitrosyl iron(II) tetraphenylporphyrin exhibits porphyrin ring ^{14}N symmetry about the Fe–N–O plane: a hyperfine sublevel correlation spectroscopy study, D.C. Gilbert and D.C. Doetschman 269 (2001) 125

Molecular spectroscopy
Higher excited state fluorescence of mixed ligand lanthanide(III) complexes with acetylacetonato, nitrate and terpyridine, M. Hasegawa, A. Nakao, M. Masui, T. Tamura, D. Suzuki, W. Linert, Y. Fukuda and T. Hoshi 269 (2001) 323
Photophysical properties of pheophorbide-*a*-substituted diaminobutane poly-propylene-imine dendrimer, S. Hackbarth, V. Horneffer, A. Wiehe, F. Hillenkamp and B. Röder 269 (2001) 339

-microwave
Calculation of ^{14}N and ^{35}Cl quadrupole coupling constants on optimized molecular structures of pyrimidine, 2-X- and 5-X-pyrimidine, with X = F, Cl, Br, and CN, W.C. Bailey 269 (2001) 75

-UV
Degeneracy, orientational disorder and chromophore size effects on Frenkel excitons in columnar mesophases, D. Markovitsi, L.K. Gallos, J.P. Lemaistre and P. Argyrakis 269 (2001) 147
Diagnosis of a benzene discharge with a mass-selective spectroscopic technique, F. Güthe, H. Ding, T. Pino and J.P. Maier 269 (2001) 347

-visible
Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results, A.A. Voityuk, A.D. Kummer, M.-E. Michel-Beyerle and N. Rösch 269 (2001) 83
Thermally induced spectral diffusion of Rhodamine 3B in viscous polyols, J.A.B. Ferreira and S.M.B. Costa 269 (2001) 313
Characterization of bisazo compounds employing ultrafast spectroscopy, R. Karpicz, V. Gulbinas, A. Stanishauskaite and A. Undzenas 269 (2001) 357

Photon counting and phase fluorimetry
Decay dynamics of interchain excited states in luminescent conjugated polymer CN-PPV, J.-H. Hsu, W. Fann, H.-F. Meng, E.-S. Chen, E.-C. Chang, S.-A. Chen and K.-W. To 269 (2001) 367

Multiphoton ionization
Diagnosis of a benzene discharge with a mass-selective spectroscopic technique, F. Güthe, H. Ding, T. Pino and J.P. Maier 269 (2001) 347

Electron impact spectroscopy
An investigation of the HOMO frontier orbital electron density distributions of NH_3, the methylamines and NF_3 using DFT and electron momentum spectroscopy, C.E. Brion, J.B. Young, I.V. Litvinyuk and G. Cooper 269 (2001) 101
Core excitation and autoionising transitions from $^{1,3}\Pi_u$ states of N_2, by near threshold electron impact, D.P. Almeida, G. Dawber, S.E. Michelin and G.C. King 269 (2001) 159

Laser induced fluorescence
Solid-state optical properties of the methyl-exopyridine–anthracene rotaxane, G. Gadret, R. Zamboni, P. Schouwink, R.F. Mahrt, J. Thies, T. Loontjens and D.A. Leigh 269 (2001) 381
The collisional quenching of $CCl_2(A\,^1B_1$ and $a\,^3B_1)$ by substituted methane molecules, Y. Gao, Y. Chen, X. Ma and C. Chen 269 (2001) 389

Ultrafast measurements
Characterization of bisazo compounds employing ultrafast spectroscopy, R. Karpicz, V. Gulbinas, A. Stanishauskaite and A. Undzenas 269 (2001) 357

Multiple resonance spectroscopy
Five-coordinate nitrosyl iron(II) tetraphenylporphyrin exhibits porphyrin ring ^{14}N symmetry about the Fe–N–O plane: a hyperfine sublevel correlation spectroscopy study, D.C. Gilbert and D.C. Doetschman 269 (2001) 125

Mass spectroscopy
Photophysical properties of pheophorbide-*a*-substituted diaminobutane poly-propylene-imine dendrimer, S. Hackbarth, V. Horneffer, A. Wiehe, F. Hillenkamp and B. Röder 269 (2001) 339

X-ray, electron and neutron diffraction
Microstructure of indocyanine green J-aggregates in aqueous solution, J. Zweck and A. Penzkofer 269 (2001) 399

Objects

Bulk systems

Gases
Reduced dimensionality quantum reactive scattering calculations on the ab initio potential energy surface for the $O(^1D) + N_2O \rightarrow NO + NO$ reaction, T. Takayanagi and A. Wada 269 (2001) 37
Calculation of ^{14}N and ^{35}Cl quadrupole coupling constants on optimized molecular structures of pyrimidine, 2-X- and 5-X-pyrimidine, with X = F, Cl, Br, and CN, W.C. Bailey 269 (2001) 75
Core excitation and autoionising transitions from $^{1,3}\Pi_u$ states of N_2, by near threshold electron impact, D.P. Almeida, G. Dawber, S.E. Michelin and G.C. King 269 (2001) 159
Chemical generation of atomic iodine for chemical oxygen–iodine laser. I. Modelling of reaction systems, V. Jirásek, O. Špalek, J. Kodymová and M. Čenský 269 (2001) 167
Equilibrium dimer concentrations in gases and gas mixtures, J.W. Eerkens 269 (2001) 189
The collisional quenching of $CCl_2(A\,^1B_1$ and $a\,^3B_1)$ by substituted methane molecules, Y. Gao, Y. Chen, X. Ma and C. Chen 269 (2001) 389

Supersonic beams
Diagnosis of a benzene discharge with a mass-selective spectroscopic technique, F. Güthe, H. Ding, T. Pino and J.P. Maier 269 (2001) 347

Liquids neat
Thermally induced spectral diffusion of Rhodamine 3B in viscous polyols, J.A.B. Ferreira and S.M.B. Costa 269 (2001) 313

Liquid mixtures and solutions
Five-coordinate nitrosyl iron(II) tetraphenylporphyrin exhibits porphyrin ring ^{14}N symmetry about the Fe–N–O plane: a hyperfine sublevel correlation spectroscopy study, D.C. Gilbert and D.C. Doetschman 269 (2001) 125
Vapor–liquid equilibria of dendrimer solutions: the effect of endgroups at the periphery of dendrimer molecules, J.G. Jang and Y.C. Bae 269 (2001) 285
A Monte Carlo simulation study of solvent effect on Eu^{3+} to Nd^{3+} ion mutation, H.-S. Kim 269 (2001) 295
Ultrasonic studies of dynamics of critical concentration fluctuations in benzonitrile–isooctane mixture, T. Hornowski and D. Madej 269 (2001) 303

Characterization of bisazo compounds employing ultrafast spectroscopy, R. Karpicz, V. Gulbinas, A. Stanishauskaite and A. Undzenas 269 (2001) 357

Crystals
Molecular dynamics studies of phase transition of KI clusters, X.-l. Zhu, X.-z. You, R.-g. Xiong and Z. Zhou 269 (2001) 243

-neat
Cobalt valence tautomeric compounds: molecular and solid state properties, S. Klokishner 269 (2001) 411

Complex fluids

-liquid crystals
Degeneracy, orientational disorder and chromophore size effects on Frenkel excitons in columnar mesophases, D. Markovitsi, L.K. Gallos, J.P. Lemaistre and P. Argyrakis 269 (2001) 147

Polymers
Decay dynamics of interchain excited states in luminescent conjugated polymer CN-PPV, J.-H. Hsu, W. Fann, H.-F. Meng, E.-S. Chen, E.-C. Chang, S.-A. Chen and K.-W. To 269 (2001) 367

Plasmas
Diagnosis of a benzene discharge with a mass-selective spectroscopic technique, F. Güthe, H. Ding, T. Pino and J.P. Maier 269 (2001) 347

Microscopic and mesoscopic systems

Molecules (neutral and ionic)
A theoretical study on electron donor–acceptor complexes of Et_2O, Et_2S and Me_3N with interhalogens, I–X (X = Cl and Br), S.P. Ananthavel and M. Manoharan 269 (2001) 49
Five-coordinate nitrosyl iron(II) tetraphenylporphyrin exhibits porphyrin ring ^{14}N symmetry about the Fe–N–O plane: a hyperfine sublevel correlation spectroscopy study, D.C. Gilbert and D.C. Doetschman 269 (2001) 125
A theoretical study of the reaction of hypochlorous acid with the bromite ion, S. Guha and J.S. Francisco 269 (2001) 179
Vapor–liquid equilibria of dendrimer solutions: the effect of endgroups at the periphery of dendrimer molecules, J.G. Jang and Y.C. Bae 269 (2001) 285
Ultrasonic studies of dynamics of critical concentration fluctuations in benzonitrile–isooctane mixture, T. Hornowski and D. Madej 269 (2001) 303
Photophysical properties of pheophorbide-*a*-substituted diaminobutane poly-propylene-imine dendrimer, S. Hackbarth, V. Horneffer, A. Wiehe, F. Hillenkamp and B. Röder 269 (2001) 339
Theoretical study TPA properties of a series of two-dimensional charge-transfer derivatives, Y.-f. Zhou, F.-q. Meng, X. Zhao, S.-y. Feng and M.-h. Jiang 269 (2001) 441

-diatomic
Finite-field Møller–Plesset perturbation theory and coupled cluster calculations of the electric multipole moments and the dipole polarizability of As_2, G. Maroulis and P. Karamanis 269 (2001) 137

Core excitation and autoionising transitions from $^{1,3}\Pi_u$ states of N_2, by near threshold electron impact, D.P. Almeida, G. Dawber, S.E. Michelin and G.C. King 269 (2001) 159

-small polyatomics

Ab initio investigation of the potential energy surfaces involved in the photophysics of s-*trans*-1,3-butadiene, B. Ostojić and W. Domcke 269 (2001) 1

Hydrogen bonding in picolinic acid *N*-oxide. Part II: A proposal for dissipative laser driven proton transfer dynamics, N. Došlić, J. Stare and J. Mavri 269 (2001) 59

An investigation of the HOMO frontier orbital electron density distributions of NH_3, the methylamines and NF_3 using DFT and electron momentum spectroscopy, C.E. Brion, J.B. Young, I.V. Litvinyuk and G. Cooper 269 (2001) 101

-aromatics

The additivity of the π-electron correlation energy in planar heteroatomic molecules, Z.B. Maksić, D.M. Smith and D. Barić 269 (2001) 11

Diagnosis of a benzene discharge with a mass-selective spectroscopic technique, F. Güthe, H. Ding, T. Pino and J.P. Maier 269 (2001) 347

-other large

Thermally induced spectral diffusion of Rhodamine 3B in viscous polyols, J.A.B. Ferreira and S.M.B. Costa 269 (2001) 313

Characterization of bisazo compounds employing ultrafast spectroscopy, R. Karpicz, V. Gulbinas, A. Stanishauskaite and A. Undzenas 269 (2001) 357

-polymeric and biological

Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results, A.A. Voityuk, A.D. Kummer, M.-E. Michel-Beyerle and N. Rösch 269 (2001) 83

Molecular aggregates

On electrodynamics of extended multiphonon transitions and nature of the J-band, V.V. Egorov 269 (2001) 251

Microstructure of indocyanine green J-aggregates in aqueous solution, J. Zweck and A. Penzkofer 269 (2001) 399

-dimers

Equilibrium dimer concentrations in gases and gas mixtures, J.W. Eerkens 269 (2001) 189

-van der Waals molecules

Potential coupling of intramolecular to intermolecular modes: an ab initio study of the amino inversion and van der Waals motions in the aniline–argon complex, I. López-Tocón, J.C. Otero, M. Becucci, G. Pietraperzia, E. Castellucci and P. Bréchignac 269 (2001) 29

-complexes

A theoretical study on electron donor–acceptor complexes of Et_2O, Et_2S and Me_3N with interhalogens, I–X (X = Cl and Br), S.P. Ananthavel and M. Manoharan 269 (2001) 49

Higher excited state fluorescence of mixed ligand lanthanide(III) complexes with acetylacetonato, nitrate and terpyridine, M. Hasegawa, A. Nakao, M. Masui, T. Tamura, D. Suzuki, W. Linert, Y. Fukuda and T. Hoshi 269 (2001) 323

Cobalt valence tautomeric compounds: molecular and solid state properties, S. Klokishner 269 (2001) 411

Free radicals (incl. hydronium and muonium)
The collisional quenching of CCl_2(A $^1B_1$ and a $^3B_1$) by substituted methane molecules, Y. Gao, Y. Chen, X. Ma and C. Chen 269 (2001) 389

Supramolecular assemblies (incl. nanoparticles and nanostructures)
Degeneracy, orientational disorder and chromophore size effects on Frenkel excitons in columnar mesophases, D. Markovitsi, L.K. Gallos, J.P. Lemaistre and P. Argyrakis 269 (2001) 147
Solid-state optical properties of the methyl-exopyridine–anthracene rotaxane, G. Gadret, R. Zamboni, P. Schouwink, R.F. Mahrt, J. Thies, T. Loontjens and D.A. Leigh 269 (2001) 381

Phenomena

Molecular structure
Calculation of ^{14}N and ^{35}Cl quadrupole coupling constants on optimized molecular structures of pyrimidine, 2-X- and 5-X-pyrimidine, with X = F, Cl, Br, and CN, W.C. Bailey 269 (2001) 75

Vibrations and rotations of molecules
The influence of the stretch modes on the classical highly excited bend motion with Darling–Dennison coupling in acetylene, G. Wu 269 (2001) 93

Electronic structure and states
Ab initio investigation of the potential energy surfaces involved in the photophysics of s-*trans*-1,3-butadiene, B. Ostojić and W. Domcke 269 (2001) 1
The additivity of the π-electron correlation energy in planar heteroatomic molecules, Z.B. Maksić, D.M. Smith and D. Barić 269 (2001) 11
Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results, A.A. Voityuk, A.D. Kummer, M.-E. Michel-Beyerle and N. Rösch 269 (2001) 83
An investigation of the HOMO frontier orbital electron density distributions of NH_3, the methylamines and NF_3 using DFT and electron momentum spectroscopy, C.E. Brion, J.B. Young, I.V. Litvinyuk and G. Cooper 269 (2001) 101
Core excitation and autoionising transitions from $^{1,3}\Pi_u$ states of N_2, by near threshold electron impact, D.P. Almeida, G. Dawber, S.E. Michelin and G.C. King 269 (2001) 159
Higher excited state fluorescence of mixed ligand lanthanide(III) complexes with acetylacetonato, nitrate and terpyridine, M. Hasegawa, A. Nakao, M. Masui, T. Tamura, D. Suzuki, W. Linert, Y. Fukuda and T. Hoshi 269 (2001) 323
Theoretical study TPA properties of a series of two-dimensional charge-transfer derivatives, Y.-f. Zhou, F.-q. Meng, X. Zhao, S.-y. Feng and M.-h. Jiang 269 (2001) 441

Electric and magnetic properties
Non-orthogonal orbitals for localized electrons III. Application to periodic one dimensional lattices, G. Bignonneau, A. Fritsch and L. Ducasse 269 (2001) 107

Finite-field Møller–Plesset perturbation theory and coupled cluster calculations of the electric multipole moments and the dipole polarizability of As_2, G. Maroulis and P. Karamanis 269 (2001) 137
Cobalt valence tautomeric compounds: molecular and solid state properties, S. Klokishner 269 (2001) 411

Molecular interactions
A theoretical study on electron donor–acceptor complexes of Et_2O, Et_2S and Me_3N with interhalogens, I–X (X = Cl and Br), S.P. Ananthavel and M. Manoharan 269 (2001) 49
Equilibrium dimer concentrations in gases and gas mixtures, J.W. Eerkens 269 (2001) 189
A Monte Carlo simulation study of solvent effect on Eu^{3+} to Nd^{3+} ion mutation, H.-S. Kim 269 (2001) 295

Spectral bandshapes and intensities
On electrodynamics of extended multiphonon transitions and nature of the J-band, V.V. Egorov 269 (2001) 251
Thermally induced spectral diffusion of Rhodamine 3B in viscous polyols, J.A.B. Ferreira and S.M.B. Costa 269 (2001) 313
Characterization of bisazo compounds employing ultrafast spectroscopy, R. Karpicz, V. Gulbinas, A. Stanishauskaite and A. Undzenas 269 (2001) 357

Coupling of electronic and nuclear motion
On electrodynamics of extended multiphonon transitions and nature of the J-band, V.V. Egorov 269 (2001) 251

Energy transfer processes
Equilibrium dimer concentrations in gases and gas mixtures, J.W. Eerkens 269 (2001) 189
Solid-state optical properties of the methyl-exopyridine–anthracene rotaxane, G. Gadret, R. Zamboni, P. Schouwink, R.F. Mahrt, J. Thies, T. Loontjens and D.A. Leigh 269 (2001) 381

Molecular photophysical processes
Decay dynamics of interchain excited states in luminescent conjugated polymer CN-PPV, J.-H. Hsu, W. Fann, H.-F. Meng, E.-S. Chen, E.-C. Chang, S.-A. Chen and K.-W. To 269 (2001) 367

Photochemistry
Ab initio investigation of the potential energy surfaces involved in the photophysics of s-*trans*-1,3-butadiene, B. Ostojić and W. Domcke 269 (2001) 1

Intramolecular dynamics
Potential coupling of intramolecular to intermolecular modes: an ab initio study of the amino inversion and van der Waals motions in the aniline–argon complex, I. López-Tocón, J.C. Otero, M. Becucci, G. Pietraperzia, E. Castellucci and P. Bréchignac 269 (2001) 29

-vibrational energy redistribution (incl. vibrational dissociation)
Hydrogen bonding in picolinic acid *N*-oxide. Part II: A proposal for dissipative laser driven proton transfer dynamics, N. Došlić, J. Stare and J. Mavri 269 (2001) 59

Luminescence spectra, yields and lifetimes
Photophysical properties of pheophorbide-*a*-substituted diaminobutane poly-propylene-imine dendrimer, S. Hackbarth, V. Horneffer, A. Wiehe, F. Hillenkamp and B. Röder 269 (2001) 339
Solid-state optical properties of the methyl-exopyridine–anthracene rotaxane, G. Gadret, R. Zamboni, P. Schouwink, R.F. Mahrt, J. Thies, T. Loontjens and D.A. Leigh 269 (2001) 381

Nonlinear responses (incl. optical)
Theoretical study TPA properties of a series of two-dimensional charge-transfer derivatives, Y.-f. Zhou, F.-q. Meng, X. Zhao, S.-y. Feng and M.-h. Jiang 269 (2001) 441

Reactions (incl. dissociation)
Reduced dimensionality quantum reactive scattering calculations on the ab initio potential energy surface for the $O(^1D) + N_2O \rightarrow NO + NO$ reaction, T. Takayanagi and A. Wada 269 (2001) 37
A theoretical study of the reaction of hypochlorous acid with the bromite ion, S. Guha and J.S. Francisco 269 (2001) 179

-collisional
Reduced dimensionality quantum reactive scattering calculations on the ab initio potential energy surface for the $O(^1D) + N_2O \rightarrow NO + NO$ reaction, T. Takayanagi and A. Wada 269 (2001) 37
Chemical generation of atomic iodine for chemical oxygen–iodine laser. I. Modelling of reaction systems, V. Jirásek, O. Špalek, J. Kodymová and M. Čenský 269 (2001) 167
The collisional quenching of $CCl_2(A\,^1B_1$ and $a\,^3B_1)$ by substituted methane molecules, Y. Gao, Y. Chen, X. Ma and C. Chen 269 (2001) 389

-condensed phase
Solid-state optical properties of the methyl-exopyridine–anthracene rotaxane, G. Gadret, R. Zamboni, P. Schouwink, R.F. Mahrt, J. Thies, T. Loontjens and D.A. Leigh 269 (2001) 381

Electron transfer
On electrodynamics of extended multiphonon transitions and nature of the J-band, V.V. Egorov 269 (2001) 251
Cobalt valence tautomeric compounds: molecular and solid state properties, S. Klokishner 269 (2001) 411

Proton and hydrogen atom transfer
Hydrogen bonding in picolinic acid *N*-oxide. Part II: A proposal for dissipative laser driven proton transfer dynamics, N. Došlić, J. Stare and J. Mavri 269 (2001) 59
Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results, A.A. Voityuk, A.D. Kummer, M.-E. Michel-Beyerle and N. Rösch 269 (2001) 83

Ionization (incl. Rydberg states)
An investigation of the HOMO frontier orbital electron density distributions of NH_3, the methylamines and NF_3 using DFT and electron momentum spectroscopy, C.E. Brion, J.B. Young, I.V. Litvinyuk and G. Cooper 269 (2001) 101

Collective motion and excitations
Degeneracy, orientational disorder and chromophore size effects on Frenkel excitons in columnar mesophases, D. Markovitsi, L.K. Gallos, J.P. Lemaistre and P. Argyrakis 269 (2001) 147

Thermodynamic and transport properties
Molecular dynamics studies of phase transition of KI clusters, X.-l. Zhu, X.-z. You, R.-g. Xiong and Z. Zhou 269 (2001) 243

Structure of solids, liquids and gases
A Monte Carlo simulation study of solvent effect on Eu^{3+} to Nd^{3+} ion mutation, H.-S. Kim 269 (2001) 295
Microstructure of indocyanine green J-aggregates in aqueous solution, J. Zweck and A. Penzkofer 269 (2001) 399

Molecular self-assembly and -organization
Microstructure of indocyanine green J-aggregates in aqueous solution, J. Zweck and A. Penzkofer 269 (2001) 399